Combined Synchrotron X-ray Diffraction Studies to Synthetic Gallogermanate Cancrinite: 2. Resonant Powder Diffraction Studies

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Beamline(s): **X7A**

Our approach to resolving the issue of Ga/Ge-ordering in the framework T-site of the gallogermanate cancrinite was to use resonant diffraction near the Ga or Ge absorption edge, and thereby introduce a scattering contrast between the two T-sites. This contrast increases from 1.03:1 for the off-edge data to 1.50:1 for the Ga K-edge data (10367 eV, f'_{Ga} = -11.68, f'_{Ge} = -2.40). Calculations using the DLS-minimized GaGe-CAN structure model and the anomalous scattering factors at the Ga K-edge indicated that the intensities of the *hh*$\bar{2}$*hl* reflections with *l* = 2n +1 would increase to as much as 1.6% of the strongest (*0002*) reflection; 1.0% when the calculation is performed at the Ge K-edge (11103 eV, f'_{Ga} = -1.87, f'_{Ge} = -10.41). The scattering contrast expected from neutron diffraction (b_{Ge} = 0.82, b_{Ga} = 0.72 pm) is less than that from resonant diffraction at the Ga K-edge (1.14:1 compared to 1.50:1), and the calculated intensities of the *hh*$\bar{2}$*hl* reflections with *l* = 2n + 1 would only be 0.8% of the strongest (*12*$\bar{3}$*1)* reflection. Resonant diffraction near the Ga K-edge was therefore chosen to observe a set of the *hh*$\bar{2}$*hl* reflections with *l* = 2n +1. The on-edge scan was performed at 10380 eV (λ = 1.1943 Å) over the (*11*$\bar{2}$*1*) and (*33*$\bar{6}$*1)* reflections. These reflections are clearly observed, with the observed intensities of these reflections close to 2.8 and 1.1% of the strongest (*0002*) reflection, respectively [1]. This establishes the space group **P**6_3 and the ordering of the Ga/Ge atoms in the T-sites of GaGe-CAN (***see X7B section***).

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References: [1] Y. Lee, J. B. Parise, A. Tripathi, S. J. Kim, and T. Vogt. (2000) Microporous Mesoporous Mater., 39, 445.

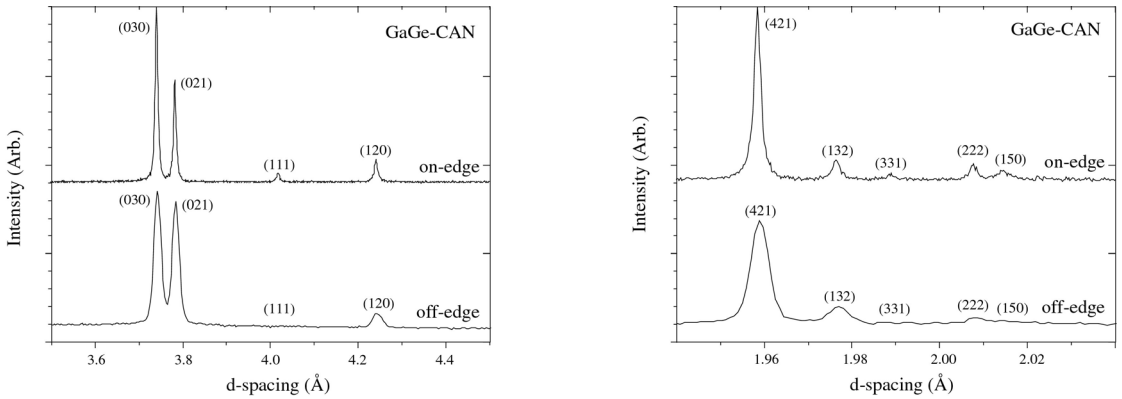

Figure. Synchrotron X-ray powder diffraction patterns scanned over the (*11*$\bar{2}$*1*) and (*33*$\bar{6}$*1)* reflections of GaGe-CAN at two different wavelengths.